p-adic description of characteristic relaxation in complex systems

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Abstract. This work is a further development of an approach to the description of relaxation processes in complex systems on the basis of the p-adic analysis. We show that three types of relaxation fitted into the Kohlrausch-Williams-Watts law, the power decay law, or the logarithmic decay law, are similar random processes. Inherently, these processes are ultrametric and are described by the p-adic master equation. The physical meaning of this equation is explained in terms of a random walk constrained by a hierarchical energy landscape. We also discuss relations between the relaxation kinetics and the energy landscapes.

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1. Introduction.

One of the distinctive features of complex systems (such as glasses, macromolecules, and proteins) is an anomalously slow non-exponential relaxation observed in a very wide range of time scales — from that of short-time molecular vibrations to days and months. Relaxation kinetics in complex systems is often fitted into three empirical laws, namely, the stretched exponential curve (the Kohlrausch-Williams-Watts law), $\sim \exp\left[-\left(t/\tau\right)^{\alpha}\right]$, $0<\alpha<1$, the power decay law, $\sim \left(t/\tau\right)^{-\alpha}$, $0<\alpha$, and the logarithmic decay law, $\sim \alpha\left[ln\left(t/\tau\right)\right]^{-1}$, $1<\alpha$ [1, 2, 3]. These types of relaxation are characteristic of complex systems, just as exponential relaxation is typical for gases and liquids.

Although formulation of a microscopic theory of anomalous relaxation in complex systems remains an issue of the day, there exist important concepts regarding the general relaxation behavior of complex systems. The starting point of these concepts is that the states of a micro-component of a system are strongly coupled to configurational rearrangements of the local environment, and it is important that these rearrangements cover a wide range of scales – from microscopic to mesoscopic. In order to describe configurational dynamics of this kind, the concept of energy landscapes is applied [4]-[11]. According to this concept, configurational rearrangements are described by a random walk in the space of configurational states, and this process, in its turn, is determined by the energy landscape of the system.

There is common understanding of the fact that a comprehensive description of energy landscapes of complex systems is hardly possible for several reasons. First of all, due to an uncertainty while selecting local potentials of interaction between the system's components. Another reason is the large number of metastable configurations, which occur due to multiple quenched constraints and the random nature of the local arrangement. The number of metastable configurations grows exponentially with respect to the size of the system. Thus, energy landscapes of mesoscopic systems (these systems are of the main interest) form multidimensional surfaces with an extremely large number of local minima. It is not quite clear how to describe those surfaces analytically and, accordingly, how to describe the configurational dynamics constrained by such landscapes. In this connection, computer simulation of model systems remains the main field of activity. These studies show that energy landscapes of complex systems may vary significantly. However, the characteristic types of relaxation obviously suggest that such landscapes have some common features. These features might turn out to be as fundamental for the dynamics of complex systems as the space symmetry is for crystal structures.

One of the nontrivial assumptions, which initially appeared in the theory of spin glasses [12] - [14], was that the energy landscapes of complex systems have a hierarchical structure. In recent years, this conjecture was confirmed by the results of numerous computer simulation studies (see, for example, [9, 15]). It turned out that energy landscapes of complex systems represent hierarchically nested basins of local minima, viz., large basins consist of smaller basins of minima, the latter consist of even smaller ones, etc. The basins of minima are separated from one another by a hierarchy of activation barriers, i.e., the larger basins are separated by higher activation barriers, while the smaller basins within the larger ones are separated by smaller activation barriers, respectively.

The existence of the basins of local minima allows one to describe configurational dynamics in terms of the basin-to-basin kinetics [9]. In this connection, it is assumed

that transitions between the basins belonging to the same level of the basin's hierarchy correspond to configurational rearrangements of a certain scale. Within such basins, a quasi-equilibrium distribution is established during relatively short (for a given scale) period of time, while transitions between the basins determine long-time configurational rearrangements. The hierarchy of nested basins corresponds to the hierarchy of scales of configurational rearrangements.

As indicated in the early works on the spin-glass theory, the hierarchy of nested basins of local minima is similar to the hierarchy of nested ultrametric spheres [12]-[14]. This idea can be found in some publications about anomalous relaxation in glass-like systems [16]-[19]. However, these investigations give no answer to the question whether ultrametricity can be directly used for the description of the dynamics of complex systems.

Recent studies [20, 21] show that there is an approach which may lead to a noticeable progress in this direction. This approach is based on the p-adic analysis natural for ultrametric spaces. An introduction to the p-adic analysis can be found, for instance, in [22]. Some applications of the p-adic analysis in theoretical physics and theoretical biology are described in [23]-[26].

The p-adic master equation describing a random walk constrained by the hierarchical energy landscapes of a certain type (the so-called ultrametric diffusion) was constructed in [20, 21]. In these works, we describe a general method of finding its solutions and examine some Cauchy problems pertaining to conformational dynamics and reactions in proteins, and we also find some solutions of these problems expressed by analytic formulas. It is an interesting fact that the p-adic pseudo-differential equation introduced earlier as a p-adic analogue of the diffusion equation (see [22]) coincides with the particular p-adic master equation obtained in [20, 21].

Regarding p-adic pseudo-differential equations and stochastic processes in non-Archimedean spaces, see [22], [27]-[29].

The present paper is aimed at a further development of the approach suggested in [20, 21] for the description of configurational dynamics of complex systems. We show that the Kohlrausch-Williams-Watts law, the power decay law, and the logarithmic decay law can be described by p-adic master equations of the same form, and therefore, the relaxation laws characteristic of complex systems actually reflect the same type of ultrametric random processes.

The paper is structured as follows. In Section 2, we introduce a general form of the p-adic master equation describing random walk constrained by a hierarchical energy landscape, and we also define a p-adic model of relaxation. In Section 3, we consider three versions of such models and establish their correspondence with three types of relaxation in complex systems.

2. Random walk in ultrametric space

The general p-adic master equation describing a Markovian process of random walk in ultrametric space can be written as follows:

$$\frac{\partial f(x,t)}{\partial t} = \int_{\mathbb{Q}_p} \left[w(x|y)f(y,t) - w(y|x)f(x,t)\right] d\mu(y), \tag{1}$$

where x is a p-adic number, $d\mu(x)$ is the Haar measure on the field of p-adic numbers $\mathbb{Q}_p$, and t is time, $t \in \mathbb{R}_+$. Equation (1) is the usual balance equation for transitions between system states. The only peculiarity is that the space

of states is described by the p-adic numbers, i.e. this space is ultrametric. The function $f(x,t) : \mathbb{Q}_p \times \mathbb{R}_+ \mapsto \mathbb{R}_+$ is a probability density distribution: the integral $\int_B f(x,t)d\mu(x)$ is the probability of finding the system in a domain $B \subseteq \mathbb{Q}_p$ at the instant t. The function $w(x|y) : \mathbb{Q}_p \times \mathbb{Q}_p \mapsto \mathbb{R}_+$ is the probability of the transition from the state y to the state x per unit time.

The transition from a state y to a state x can be perceived as overcoming the energy barrier separating these states. The structure of the relation between the transition probability $w(x|y)$ and the parameters of the energy barrier depends, in general, on the mechanism of configurational rearrangements, transition pathways, their distribution, etc. Finding this expression on the basis of the microscopic theory is a nontrivial problem beyond the scope of this article. For the sake of definiteness, we will use the standard Arrhenius relation

$$w(x|y) \sim A(T) \exp\left\{-\frac{U(x|y)}{kT}\right\} \tag{2}$$

where $U(x|y)$ is the height of the (effective) activation barrier for the transition from the state y to the state x, k is the Boltzmann constant, and T is temperature. Studies of thermal behavior of anomalous relaxation in complex systems show that this expression is quite acceptable for a fairly wide range of temperatures.

Formula (2) establishes a relation between the structure of the energy landscape $U(x|y)$ and the transition function $w(x|y)$. In particular, the condition $w(x|y) = w(y|x)$ corresponds to a degenerate energy landscape. An important example of a degenerate landscape is a regular hierarchical landscape. In this case, on each hierarchical level, the basins of states split up into the same number of smaller basins; moreover, the activation barriers between the basins of the same hierarchical level have equal values. Graphically, this hierarchical landscape is represented as a regular tree with the same branching rules for all branching nodes. As shown in [20, 21], the activation barriers $U(x|y)$ separating the states x and y depend, in this case, only on ultrametric distances between the states, $|x-y|_p = p^{\gamma}$, $\gamma \in \mathbb{Z}$, and therefore, regular energy landscapes are completely described by functions of the form $U(|x-y|_p)$. Thus, in the case of random walk constrained by a regular hierarchical landscape, the master equation (1) takes the form

$$\frac{\partial f(x,t)}{\partial t} = \int_{\mathbb{Q}_p} W(|x-y|_p)\left[f(y,t) - f(x,t)\right] d\mu(y) \tag{3}$$

where

$$W(|x-y|_p) = \frac{A(T)}{|x-y|_p} \exp\left\{-\frac{U\left(|x-y|_p\right)}{kT}\right\} .$$

The p-adic master equation (3) admits analytic solutions for a fairly wide class of functions $W(|x-y|_p)$. The technique of finding its solutions is described, for instance, in [20, 21].

It may seem that regular hierarchical landscapes represent a very idealistic model of real landscapes and have little relation to the latter. Indeed, regular hierarchical landscapes reflect no details of the energy landscapes of complex systems other than their hierarchical structure. Oddly enough, this is sufficient for the description of the characteristic types of relaxation.

On the basis of general physical considerations, one can identify three essentially different types of regular hierarchical landscapes:

"Logarithmic landscapes" are characterized by activation barriers having a slow (logarithmic) growth with respect to the number γ of the hierarchical level, $U(\gamma) \sim \ln \gamma$. This type of landscapes may be associated with "flexible" systems having a wide range of available scales for configurational rearrangements.

Contrary to logarithmic landscapes, "exponential landscapes" are characterized by a rapid (exponential) growth of activation barriers, $U(\gamma) \sim e^{\gamma}$. Landscapes of this type represent "stiff" systems with a small set of distinct scales available for configurational rearrangements.

Finally, there are "linear landscapes" with linear growth of activation barriers, $U(\gamma) \sim \gamma$. These landscapes may be associated with systems of an "intermediate" type.

In all these cases, we consider the Cauchy problem for the respective master equation (3) with the initial conditions:

$$f(x,0) = \Omega\left(|x|_p\right) = \begin{cases} 1 & |x|_p \leq 1 \\ 0 & |x|_p > 1 \ . \end{cases} \tag{4}$$

A relaxation process will be understood as the evolution of population in the domain of the initial distribution $|x|_p \leq 1$:

$$S(t) = \int\limits_{|x|_p \leq 1} f(x,t) d\mu(x) \ . \tag{5}$$

In each of the above cases, the analytical estimation of relaxation function $S(t)$ is being found. It would enable the relation of $S(t)$ to three empirical laws for characteristic relaxation.

3. Characteristic relaxation types

The solution of the Cauchy problem for equation (3) with the initial condition (4) has the form

$$f(x,t) = \sum_{n=0}^{\infty} e^{\tilde{W}(p^{-n})t} \left[(1-p^{-1})p^{-n}\Omega(p^{-n}\,|x|_p) - p^{-n-1}\delta(|x|_p - p^{1+n})\right] \tag{6}$$

where

$$\delta(|x|_p - p^{\gamma}) = \begin{cases} 1 & |x|_p = p^{\gamma} \\ 0 & |x|_p \neq p^{\gamma} \ . \end{cases}$$

Indeed, applying the p-adic Fourier transformation to (3) and taking into account the initial condition (4), we get

$$f(x,t) = \int_{\mathbb{Z}_p} e^{\tilde{W}(|k|_p)t} \chi(-kx) d\mu(k)$$

where

$$\tilde{W}(|k|_p) = \int_{\mathbb{Q}_p} W(|x|_p)(\chi(kx) - 1) d\mu(x) \ . \tag{7}$$

Calculating the integral and using the substitution $|k|_p = p^{-n}$, we obtain

$$\tilde{W}(p^{-n}) = -p^{n+1}\left[(1-p^{-1})\sum_{m=0}^{\infty} p^m W(p^{m+n+1}) + p^{-1}W(p^{n+1})\right]$$

and therefore, (6) is the desired solution.

In order to find $S(t)$, the solution (6) should be substituted into (5). Calculating the corresponding integral, we find that

$$S(t) = (p-1) \sum_{n=1}^{\infty} p^{-n} e^{-\Lambda_n t} \,. \tag{8}$$

Here, for the sake of convenience, we have introduced the positive function

$$\Lambda_n = p^n \left[(1-p^{-1}) \sum_{m=0}^{\infty} p^m W(p^{m+n}) + p^{-1} W(p^n) \right] . \tag{9}$$

Next, we obtain estimates of $S(t)$ for the above three regular hierarchical landscapes. The transition probability W is defined here by (2). The frequency factor is taken equal to the unity, and the temperature dependence is characterized by the parameter $\alpha = T_0 / T$.

3.1. Logarithmic landscape.

In view of (2), the transition probability function for the logarithmic landscape can be represented as

$$W(|x-y|_p) = \frac{1}{|x-y|_p} \, \frac{1}{\ln^{\alpha}(1+|x-y|_p)} \,, \quad \alpha > 1 \,.$$

In this case,

$$\Lambda_n = (1-p^{-1}) \sum_{m=0}^{\infty} \ln^{-\alpha}(1+p^{m+n}) + p^{-1} \ln^{-\alpha}(1+p^n) \,. \tag{10}$$

Then, the following estimates hold:

$$(1-p^{-1}) \frac{\ln^{-\alpha} p}{(\alpha-1)} \frac{1}{(n+1)^{\alpha-1}} < \Lambda_n < \frac{\alpha \ln^{-\alpha} p}{(\alpha-1)} \frac{1}{n^{\alpha-1}} \,.$$

Using these inequalities, we can estimate the relaxation function $S(t)$ as follows:

$$p \, \exp\left\{ -\frac{2\alpha}{\alpha-1} \left(\frac{t}{\ln p} \right)^{\frac{1}{\alpha}} \right\} < S(t) < p^2 \left(\exp\left\{ -\frac{1}{\alpha-1} \left(\frac{t}{\ln p} \right)^{\frac{1}{\alpha}} \right\} + \exp\left\{ -\left(\frac{t}{\ln p} \right)^{\frac{1}{\alpha}} \right\} \right) .$$

Thus, *the long-time behavior of relaxation kinetics constrained by logarithmic landscapes is fitted into the Kohlrausch-Williams-Watts law.*

It is interesting to note, that as $\alpha \to 1$, the upper bound for $S(t)$ approaches an exponent. For $\alpha \leq 1$, the series (10) is divergent. This fact may be interpreted as a transition to exponential relaxation when a critical temperature T_0 is attained. This kind of critical behavior of ultrametric diffusion constrained by logarithmic landscape was previously predicted in [16] on the basis of some qualitative considerations.

3.2. Linear landscape.

In the case of a linear landscape, the transition probability function has the form:

$$W(|x-y|_p) = \frac{1}{|x-y|_p^{\alpha+1}} \ .$$

Estimates for the probability density distribution $f(x,y)$ in the case of a linear landscape were obtained in [21]. Calculations for $S(t)$ similar to those of [21] yield the estimate

$$\frac{1}{p}\Gamma\left(\frac{1}{\alpha}+1\right)(-\Gamma_p(-\alpha)t)^{-\frac{1}{\alpha}} < S(t) < \Gamma\left(\frac{1}{\alpha}+1\right)(-\Gamma_p(-\alpha)t)^{-\frac{1}{\alpha}}$$

where $\Gamma(\alpha)$ is the gamma-function and $\Gamma_p(\alpha)$ is the p-adic gamma-function (see [22]).

Thus, *the long-time behavior of relaxation kinetics constrained by linear landscapes is fitted into the power decay law.*

3.3. Exponential landscape.

In this case, the transition probability function is

$$W(|x-y|_p) = \frac{1}{|x-y|_p}\ e^{-\alpha|x-y|_p} \ , \quad \alpha > 0,$$

and from (9) we have

$$\Lambda_n = \left(1-\frac{1}{p}\right)\sum_{m=0}^{\infty}\exp\left[-\alpha p^{n+m}\right] + \frac{1}{p}\ \exp\left[-\alpha p^n\right] \ .$$

The following estimates hold:

$$\exp\left[-\alpha p^n\right] < \Lambda_n < \frac{p^\alpha}{p^\alpha - 1}\exp\left[-\alpha p^n\right] \ .$$

Hence, for relaxation function $S(t)$ we get

$$\frac{p}{2e}\ \frac{\alpha}{\ln t + \ln\left(p^\alpha/(p^\alpha-1)\right)} < S(t) < (p^2+p+e)\frac{\alpha}{\ln t} \ .$$

The last estimate shows that *the long-time behavior of relaxation kinetics constrained by exponential landscapes is fitted into the logarithmic decay law.*

It has been shown that the Kohlrausch-Williams-Watts law, the power decay and the logarithmic decay laws reflect the same type of random processes. Such processes are ultrametric and can be described by the p-adic master equation formulated in [20, 21]. It seems that ultrametricity is a most general and fundamental feature of the dynamics of complex systems: The configurational space of such systems may be totally disconnected due to numerous quenched constraints, and therefore, it is impossible to accomplish a relatively large configurational rearrangement step-by-step, by way of small configurational changes.

In conclusion, we consider it necessary to make a few remarks.

A direct comparison of the function $S(t)$ with experimentally observed relaxation kinetics requires a certain caution. Indeed, the function $S(t)$ is the population of a region in the configurational space, whereas in most experiments, the focus of observation is some probe coupled to configurational rearrangements, rather than configurational rearrangements themselves. A specific form of the relation between the probe state and a local configuration may happen to be important for the description of experimental data.

The above three characteristic relaxation laws do not exhaust the diversity of relaxation kinetics in complex systems. There are numerous observations of "mixed" types of kinetics, with one type of relaxation kinetics observed in some time-window and another type observed outside. For instance, it may happen that at low temperatures the observed kinetics is well fitted into the logarithmic decay law, and at higher temperatures it is described by the power decay law. In other cases, the power decay may transform into the Kohlrausch-Williams-Watts law. It is not difficult to imagine energy landscapes whose activation barriers near the ground state are close to the exponential landscapes, while higher activation barriers correspond to a linear landscape and then transform into a logarithmic landscape. The above approach can be easily used for the description of ultrametric diffusion constrained by such "mixed" landscapes. Equation (3) can be solved analytically for a wide class of functions $W(|x-y|_p, \alpha)$ admitting the p-adic Fourier transformation.

Finally, our considerations here are restricted to degenerate energy landscapes. These may be directly related only to some specific complex systems, for example, spin glasses. However, energy landscapes of other complex systems are obviously non-degenerate. Local minima in such landscapes are also clustered into a hierarchy of basins, and as the whole, they look like a global potential “hole” (or “funnel”) with extremely rugged “walls”. The description of random walk on such landscapes by p-adic equations is of great interest, particularly, in connection with the applications of the concept of hierarchical energy landscapes to the protein folding [30] (see also [31] and references therein). Some results regarding this problem will be presented in our further publications.

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